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Project Summary

Environmental Hazard Rankings of Pollutants Generated in Coal Gasification Processes

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This report evaluates and ranks environmental hazards associated with coal gasification. The chemical analytical data applied toward this end have been provided through research conducted with an experimental gasifier at Research Triangle Institute, and by sampling at four commercial gasification processes by Radian Corporation. Gas, liquid, tar, and solid streams have been quantitatively analyzed for almost 300 substances. Levels of production, stream concentrations, and estimated hazard potential of individual substances are included. Hazard potential is measured utilizing a methodology developed by Research Triangle Institute and the Environmental Protection Agency, IERL-RTP.

A "worst case" approach has been taken in this summary, with maximum stream concentrations emphasized for all processes. These processes represent packed-bed, low- to medium-Btu gasifiers, which are known to produce significant contaminant loadings relative to other gasifiers. Coals tested ranged from lignite to anthracite. A representative group of approximately 50 pollutants has been emphasized and ranked according to relative environmental hazard potentials. Estimated relative hazard potentials have been categorized for streams and the process units investigated.

This Project Summary was developed by EPA's Industrial Environmental Research Laboratory, Research Triangle Park, NC, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

EPA's Industrial Environmental Research Laboratory (EPA/IERL-RTP) has sponsored and continues to direct a comprehensive environmental assessment of coal gasification processes. Over the past 4 years, emphasis has been on generation of new data for assessment. This program has been concerned with developing methods of analyzing environmental assessment data as well as with the actual experimental and source sampling aspects of assessment.

The following summary of some assessment results addresses potentially hazardous chemical species derived from various industrial and experimental coal gasification operations. The data summarized are taken from a source report[1] which contains: a) tabulated chemical analysis results for individual product/byproduct, process, and waste streams for the processes described; b) basic process information such as coal types, feed and product flow rates, and heating values; and c)

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listings of streams tested, with flow rates, and indices computed which indicate total stream potential hazard in terms of both concentrations and mass flow levels. The data compilation, evaluation, and results of this summary rank gasification pollutants in terms of their environmental hazard potential and control priorities.

The process streams and effluents characterized vary considerably in their physical and chemical natures and quantities. Therefore, a systematic approach was required to analyze the results on a common basis for comparison and/or ranking. The approach used here for comparing different chemical species on the basis of their potential environmental hazard is the Multimedia Environmental Goals (MEGs) method.

MEGs[2] (developed under a separate EPA/IERL-RTP program) are estimated or regulated levels of maximum chemical concentrations which can exist in the environment without posing health or ecological hazards. Ambient level MEG values (AMEGs) represent approximate concentrations (e.g., in μg pollutant/m^3 air) of contaminants in the ambient air, water, or land, below which unacceptable negative effects to the surrounding populations or ecosystems do not occur. Discharge MEGs (DMEGs) represent approximate maximum concentrations for contaminants in source emissions to air, water, or land, which will not evoke significant harmful or irreversible responses in exposed humans or the ecology when these exposures are of short duration (e.g., 8-hour periods). DMEGs for human health and ecology have been developed for use in assessing the impact of effluent discharges.[2-5] Estimated levels are based on existing chemical toxicity data and receptor models. Numerous applications of MEGs, including assessment of a variety of synthetic fuels processes, have been presented elsewhere.[6]

In this study the chemical concentrations and production levels (in several coal gasification product/byproduct, discharge, and process streams) have been compared with DMEGs. Since coal gasification plants may require up to 30,000 tons of coal per day, undesirable process stream constituents present in very low concentrations can be concentrated or accumulated to levels which are hazardous to human health or the natural environment. In assessing these hazards, however, substantial uncertainties in receptor (plants, animals) assimilation, and other complex factors affect chemical dilution and synergisms. Therefore, comparison of chemical levels with estimated, non-hazardous maxima (DMEGs) is most useful on a qualitative basis; e.g., ranking of potential hazards of different chemicals from measured concentrations.

The chemical data summarized have been obtained from: 1) four commercial-scale, packed-bed gasifiers, sampled by Radian Corporation; and 2) a laboratory coal gasification system at Research Triangle Institute. Along with process stream concentrations, levels of production of chemical species per unit coal mass feed to the gasifiers are also included.

Radian Corporation Source Tests

Radian Corporation has conducted source tests at four operating coal gasification facilities:

1. A Wellman-Galusha gasifier converting anthracite coal into fuel gas used for brick manufacturing.[7] Data from five different streams are included: gasifier ash and cyclone dust (solid waste); ash sluice water (liquid effluent); and poke hole gas and coal hopper gases (gas emissions).
2. A second Wellman-Galusha gasifier[8] converting North Dakota Indian Head lignite to low-Btu gas. Data on several different streams are included: gasifier ash and cyclone dust; cyclone quench water; ash sluice water and service water; and product gas and coal bin vent gas. Flow rates were unavailable for the coal bin vent gas.
3. A Chapman (Wilputte) gasifier converting low-sulfur, Virginia bituminous coal to low-Btu fuel gas.[9] Data on six effluent streams were available: cyclone dust; gasifier ash and byproduct tar; coal feeder vent gas and separator vent gas; and separator liquid, a recycled aqueous stream.
4. A Lurgi gasifier at Kosovo, Yugoslavia,[10-12] converting Yugoslavian lignite to medium-Btu fuel gas. A total of 18 gaseous streams (8 discharge, 10 process) and 3 liquid streams were sampled. The gaseous discharge streams were autoclave vent gas, coal bunker vent gas, CO_2-rich Rectisol gas, tar tank vent gas, medium oil tank vent gas, phenolic water tank vent gas, degassing column gas, and gasoline tank vent gas. Cyanic water and the inlet and outlet from the Phenosolvan unit are aqueous process streams that were sampled. No solid stream data were available.

The sampling strategies did not yield data that were directly comparable. Sampling was not meant to be exhaustive, but focussed on streams of potential environmental significance.

RTI Gasifier Tests[13-15]

Data from 10 selected semicontinuous fixed-bed tests with RTI laboratory gasifier were analyzed in detail. In each case, the solid gasifier ash and the aqueous condensate stream were the two discharge samples. Two additional streams, product gas and byproduct tar, were also sampled. The 10 selected tests involved steam/air gasification of North Dakota Beulah/Zap lignite; Montana Rosebud/McKay and Wyoming Smith/Roland subbituminous coals; Illinois No. 6 and Western Kentucky No. 9 bituminous coals; and Pennsylvania Bottom Red Ash anthracite.

Objectives and Approach

Objectives

This summary:

1. Distills the voluminous data from the sources described earlier, and compiled and presented in the source report.[1]
2. Presents a "worst case" evaluation of potential pollutant production problems from coal gasifiers, with gravitating or fixed-bed, low- to medium- Btu gas producers as the baseline. The gasification reactors are typical, with substantial coal being devolatilized at moderate temperatures, substantial tar production, and production of practically all constituents which can be derived from coal treatment. The commercial units represented are older (designed when environmental control was of less concern) and among the very few such processes available for on-site sampling. Tests selected for the RTI experimental gasifier represent a wide range of operating conditions, including low efficiency for fuel gas production, where pollutant output can be expected to be increased. The data thus

presented stand as a reference for other research and commercial operation planning.

3. Summarizes gasifier input and output streams in keeping with the "worst case" approach. Toward this end, maximum concentrations of constituents found in process streams are presented. The DMEGs, especially where supported by extensive toxicity data, also are representative of rather stringent control limits. While seeming to present the environmental problems of coal gasification in their worst light, this is certainly not an objective. For example, the "worst case" approach allows a high level of confidence in determining (from an extensive body of data) which constituents never present an apparent environmental hazard, and which can therefore be eliminated from future analysis and concern.
4. Ranks pollutants. Using the method of Multimedia Environmental Goals for normalization, the environmental hazards of each constituent are assessed relative to others. Emphasis is on those constituents which have shown consistent potential of environmental hazard. This relative comparison of compound hazard potential offers more well-founded, and therefore useful, results than do absolute values of the estimated severities.

Approach

From the source report, maximum concentrations of all constituents in each sampled stream were selected. The maxima obtained retain the designations associated with their sampling procedure, including the place of each in the following categories:

1. Processes—including each of the four commercial gasification plants and/or the composite of all RTI experimental data.
2. Stream classifications—
   a. *Discharge:* Streams which are likely candidates for direct disposal or which represent fugitive emissions at plant sites, for the processes considered.
   b. *Products/byproducts:* Streams which are likely to cross plant boundaries, with all or part of the constituents intended for commercial application. While these streams may be intended for further treatment or synthesis, their environmental hazard potential is based on the further handling and transportation of the raw stream.
   c. *Process:* Streams moving material from one unit operation to another within the plant boundaries.
3. Physical characteristics—Media considered are gases, liquids (aqueous), tars, and solids. Tars are considered separately from liquids because of their particular properties and likelihood of separation from other liquids in process operations.

All individual concentrations have been multiplied by their associated stream flow rates and divided by total process coal throughputs to obtain production factors (PFs) in units of micrograms of constituent (pollutant) produced per gram of coal input. Production factors serve two important purposes in evaluation of environmental hazard:

1. They allow comparison of potential stream hazards on the basis of both concentration and stream volume; e.g., a stream which appears hazardous, because of high concentration levels of certain constituents, may have a low flow rate that actually represents a very small production of those materials. The PF accounts for this.
2. They offer a normalization (production per unit coal input) which allows comparison of data obtained from units or streams of significantly different sizes.

DMEGs are applied as the environmental standard against which stream concentrations are measured. These estimated maximum, short-term concentration goals are used because, despite limitations, the MEG data base provides the most comprehensive and best supported one available for such purposes. More than 650 chemical substances and physical agents are included in the system. Primary emphasis has been on contaminants from fossil fuel processes.

In the MEG data base, each chemical species is assigned six Discharge Multimedia Environmental Goal (DMEG) and six Ambient Multimedia Environmental Goal (AMEG) values. These values represent target concentration limits for air (a), water (w), or land (l), and consider separate effects for both human health (h) and the ecology (e). In this study, the health-based DMEG values were used primarily. DMEGs allow the environmental assessment to avoid the complex considerations of prolonged exposure and possible accumulation in the environment over long terms.

When a DMEG value is not available for an identified chemical, the lowest DMEG value for the particular category of compounds into which the substance falls is generally chosen (the most conservative approach).

Discharge severity (DS) is an index of the degree to which the concentration of a particular substance is potentially hazardous in a process stream effluent.[18] DS is the concentration of a substance in a potential discharge (stream) divided by the DMEG value for that substance. A DS value exists for all DMEG values applicable to a substance's concentration. Wherever DS is ≥ 1, a potential hazard exists.

DMEG values have also been applied to the production factors (PFs) in this summary, in the simplest approach possible. An index is calculated which is referred to as Control Priority, CP = PF/DMEG. The production factor has been divided by the DMEG for health/water only for each pollutant. This allows all pollutants to be compared on the same basis without regard to stream type (gas, liquid, solid), since the PF for each pollutant is its maximum total process production for all streams in that process.

Air, water, and land DMEGs are typically related by constant factors, so that choice of $DMEG_{h,w}$ in calculating CP is a convenience which adequately reflects the relative importance of each pollutant, in terms of both its maximum process production (per unit coal converted) and its hazard potential (DMEG). The CP value obtained is in cm^3/g coal or g/g coal. Application of CP is advantageous when ranking pollutants from process to process since the ranking is normalized by unit mass of coal converted in each process.

Table 1 gives maximum concentrations and maximum production factors derived from the source report. Stream representations (discharge, product/byproduct, process), processes, discharge severity levels (both health and ecological), and identification of priority pollutants are all indicated. Table 2 lists a number of pollutants which have been

Table 1. Maximum Concentration Values in Each Stream Phase

	MEG Category	Chemical Name	Maximum Concentration (Source, Stream Type) $log_{10}DS_h/log_{10}DS_e$ Gas (µg/m³)	Liquid (µg/l)	Solid (µg/g)	Tar (µg/g)	Maximum Production Factor & Source µg/g coal	
o	01A	methane	1.1E8 (K,S)1/1	—	—	—	1.2E5	R
o	01A	ethane	2.1E7 (K,D)0/0	—	—	—	7.4E3	K
	01A	propane	1.6E5 (R,P)	—	—	—	4.2E2	R
	01A	butanes	6.5E4 (R,P)	—	—	—	1.7E2	R
	01A	n-butanes	—	—	—	—	1.7E2	R
	01A	isobutane	6.5E4 (R,P)	—	—	—	1.7E2	R
	01A	pentanes	—	—	—	—	1.2E-5	K
	01A	alkanes $>C_8$	6.4E2 (C,D)	1.0E5 (C,S)	2.0E0 (C,D)	4.0E2 (C,P)	4.9E1	C
	01A	methylcyclohexane	—	4.0E2 (C,S)	—	—	—	
	01A	alkanes $>C_{13}$	1.0E5 (C,D)	—	2.0E0 (C,D)	9.0E2 (C,D)	9.2E1	C
o	01A	C_3-hydrocarbons	1.3E7 (K,S)0/-	—	—	—	—	
o	01A	C_4-hydrocarbons	1.1E7 (K,S)1/-	—	—	—	—	
o	01A	C_5-hydrocarbons	2.9E6 (K,D,S)1/1	—	—	—	—	
o	01A	C_6-hydrocarbons	2.9E8 (K,D)2/2	—	—	—	—	
	01A/B	ethane and ethylene	—	—	—	—	1.0E-6	K
o	01B	ethylene	5.9E6 (K,S)0/5	—	—	—	6.9E3	K
	01B	propylene	1.9E5 (R,P)	—	—	—	4.9E2	R
	01C	acetylene	1.2E4 (R,P)	—	—	—	3.1E1	R
	01C	phenylacetylene	1.4E3 (C,D)	—	—	—	2.5E-1	C
	03A	anisoles	—	1.3E6 (C,S)	—	8.4E3 (C,P)	8.4E2	C
	03A	methylanisole	2.0E3 (C,D)	—	—	—	3.5E-1	C
	05A	aliphatic alcohols $>C_8$	1.5E4 (C,D)	—	—	—	3.4E2	C
	05A	aliphatic alcohols $>C_{13}$	3.1E3 (C,D)	—	—	—	6.2E-2	C
	05B	alkylalcohols $>C_8$	—	1.2E4 (C,S)	—	3.4E3 (C,P)	—	
	05B	alkylalcohols $>C_{13}$	—	5.4E3 (C,S)	—	—	—	
	07B	acetophenone	1.5E2 (C,D)	—	—	—	3.2E-2	C
	08A	phthalic acids	4.3E3 (C,D)	4.0E3 (C,S)	—	—	1.0E1	C
	08A	phthalic esters	6.8E4 (C,D)	—	—	1.0E2 (C,P)	3.0E3	C
	08D	adipate esters	4.9E4 (C,D)	1.9E4 (C,S)	3.0E0 (C,D)	2.2E4 (C,P)	2.2E3	C
o	08D	phthalate esters**	3.1E4 (C,D)1/1	2.2E4 (C,S)-/4	9.0E0 (C,D)-/1	3.0E4 (C,P)0/4	—	
	08D	$>C_8$ aliphatic esters	—	—	—	4.8E3 (C,P)-/3	4.8E2	C
	09B	cyanotoluene (benzonitrile)	1.1E3 (C,D)	—	—	—	1.6E1	C
			—	—	—	—	2.0E-1	C
o	10C	aniline	9.2E2 (C,D)	3.0E3 (C,S)-/0	—	2.7E2 (R,P)-/0	8.9E0	R
o	10C	C_2-alkylaniline	3.7E3 (C,D)	1.0E3 (C,S)-/0	—	1.0E2 (C,P)-/0	1.0E1	C
o	10C	C_3-alkylaniline	—	—	—	2.0E2 (C,P)-/0	2.0E1	C
o	10C	aminotoluene	2.7E3 (C,P)1/1	3.8E3 (C,S)0/0	—	9.0E2 (C,P)0/0	4.8E-1	C
o	10C	benzofluoreneamine	—	—	—	6.0E2 (C,P)0/0	6.0E1	C
	10C	methylaminoacenaphthylene	—	—	—	2.0E2 (C,P)	2.0E1	C
	10C	methylbenzofluoreneamine	—	—	—	2.0E2 (C,P)	2.0E1	C
+o	10C	benzidine	—	—	—	6.0E2 (R,P)-/1	2.0E1	R
o	10C	1-aminonaphthalene	2.0E3 (C,D)0/0	—	—	1.0E3 (C,P)-/2	1.0E2	C
o	10C	methylaminonaphthalene	5.4E3 (C,D)1/1	—	—	—	1.1E-1	C
o	10C	aminotetralin	—	—	—	9.0E2 (C,P)0/1	9.0E1	C
o	13A	methanethiol	1.1E7 (K,D)4/4	—	—	—	1.5E3	K
o	13A	ethanethiol	2.7E7 (K,D)4/4	—	—	—	—	
	13A	C_3H_8S	—	—	—	—	1.0E2	R
+o	15A	benzene	1.3E8 (K,D)4/6	9.0E2 (K,S)	—	—	1.0E2	R
o	15A	C_2-alkylbenzene	7.0E3 (C,D)0/0	—	1.0E0 (C,D)	—	—	
o	15A	C_3-alkylbenzene	2.3E4 (C,D)0/1	—	—	—	4.2E0	C
+o	15A	toluene	9.5E6 (K,D)1/3	5.0E2 (K,S)-/0	—	—	2.2E3	R
+	15A	ethylbenzene	8.8E4 (R,P)	—	—	—	2.3E2	R
	15A	styrene	6.2E3 (C,D)	—	—	—	1.1E0	C
	15A	C_3-benzene	4.9E4 (R,P)	—	—	—	1.2E2	
o	15A	C_4-benzene	2.5E5 (R,P)0.0	—	—	—	8.4E2	R
o	15A	biphenyl	5.1E3 (F,P)1/1	—	—	3.9E3 (R,P)0/0	9.2E1	R
o	15A	biphenylene	1.3E4 (C,D)-/2	—	—	—	—	
o	15A	diphenylmethane	2.7E3 (R,P)0/0	—	—	—	6.5E0	R
o	15A	indene	1.5E5 (C,D)0/0	8.2E3 (C,S)	—	3.0E2 (C,P)	4.4E2	R
	15B	indan	2.0E4 (C,D)	—	—	—	4.4E1	R
	15B	C_2-alkylindane	2.1E4 (C,D)	—	—	—	—	
	15B	C_3-alkylindane	3.2E4 (C,D)	—	—	—	—	

Table 1. *(Continued)*

	MEG Category	Chemical Name	Maximum Concentration (Source, Stream Type) $log_{10}DS_n/log_{10}DS_s$ Gas (µg/m³)	Liquid (µg/l)	Solid (µg/g)	Tar (µg/g)	Maximum Production Factor & Source µg/g coal	
	15B	methylindane	1.8E4 (C,D)	—	—	—	—	
o	15B	xylenes	4.8E5 (R,P)-/0	8.0E2 (K,S)	—	—	8.0E2	R
	15B	o-xylene	4.8E1 (F,P)	—	—	—	—	
	15B	m- and p-xylene	4,8E1 (F,P)	—	—	—	—	
+o	15B/A	xylene and ethyl benzene	1.3E6 (K,D)0/0	—	—	—	—	
	15B	tetrahydronaphthalene	3.3E3 (C,D)	—	—	—	6.6E2	C
+o	16A	polychlorinated biphenyls (PCB)**	1.5E1 (F,P)1/1	—	—	—	3.1E-2	FS
+o	17A	dinitrotoluenes	2.3E3 (F,P)0/0	—	—	—	4.5E0	FS
+o	18A	phenols	2.6E7 (K,D)3/3	2.8E6 (R,D)2/3	—	2.2E4 (R51,P)1/2	1.6E3	R
o	18A	C_2-alkylphenol	2.3E5 (C,D)1/1	3.7E5 (C,S)1/3	—	5.8E3 (C,P)4/2	6.8E2	C
o	18A	C_3-alkylphenol	1.8E4 (C,D)0/-	5.0E4 (C,S)0/2	—	1.0E3 (C,P)3/1	1.0E2	C
	18A	C_4-alkylphenol	2.1E3 (C,D)	—	—	—	3.8E-1	C
o	18A	isopropylphenol	—	—	—	1.4E4 (R,P)4/2	—	
	18A	o-isopropylphenol	—	—	—	—	1.7E2	R
o	18A	cresol	2.7E5 (C,D)1/1	1.5E6 (R,D)5/3	—	6.7E4 (R,P)3/3	1.6E3	R
o	18A	xylenol	6.0E5 (R,P)1/1	3.7E5 (R,D)5/3	—	1.2E5 (R,P)5/3	1.3E3	R
o	18A	2,4,6-trimethylphenol	—	1.8E4 (R,D)3/1	—	2.4E4 (R,P)4/2	—	
	18A	trimethylphenol	—	—	—	—	1.7E2	R
o	18C	1-naphthol	2.4E3 (C,D)	—	—	1.8E3 (C,P)3/1	—	
	18C	naphthol	—	—	—	—	1.8E2	C
o	18C	1-acenaphthol	—	—	—	3.0E2 (C,P)-/0	—	
o	18C	C_2-alkylacenaphthol	—	—	—	1.6E3 (C,P)3/1	—	
o	18C	C_3-alkylacenaphthol	—	—	—	7.0E2 (C,P)2/0	—	
o	18C	C_2-alkylhydroxyacenaphthene	1.5E3 (C,D)	—	—	—	1.6E2	C
	18C	C_3-alkylhydroxyacenaphthene	3.7E2 (C,D)	—	—	—	7.0E1	C
o	18C	C_3-alkylhydroxyanthracene	—	—	—	2.0E3 (C,P)3/1	2.0E2	C
	18C	C_2-alkylhydroxyprene	—	—	—	2.1E3 (C,P)	2.1E2	C
o	18C	C_2-alkylnaphthol	2.7E2 (C,D)	—	—	3.0E2 (C,P)2/0	3.0E1	C
	18C	hydroxyacenaphthylene	—	—	—	—	7.4E-3	C
	18C	hydroxyacenaphthene	7.3E2 (C,D)	—	—	—	3.0E1	C
o	18C	hydroxyanthracene	5.5E2 (C,D)	—	—	1.5E3 (C,P)3/2	1.5E2	C
o	18C	hydroxybenzofluorene	—	—	—	3.5E3 (C,P)3/1	3.5E2	C
o	18C	methylacenaphthol	—	—	—	9.0E2 (C,P)3/1	—	
o	18C	methylnaphthol	3.5E3 (C,D)	—	—	2.0E3 (C,P)-/1	2.0E2	C
	18C	methylhydroxyacenaphthene	—	—	—	—	9.0E1	C
o	18C	indanol	6.4E2 (C,D)	—	—	3.0E2 (C,P)	3.0E1	C
o	20B	dinitrocresol	1.8E4 (F,P)2/2	—	—	—	3.7E0	C
+o	21A	naphthalene	6.0E5 (R,P)1/1	1.7E4 (C,S)-/2	3.0E0 (C,D)	5.7E4 (R,P)-/3	2.3E4	R
	21A	higher aromatics	2.8E4 (K,S)	—	—	—	3.5E-1	K
	21A	methylnaphthalenes	1.9E5 (C,D)	5.1E3 (C,S)	2.0E0 (C,D)	7.9E3 (R,P)	—	
	21A	1-methylnaphthalene	1.2E3 (R,P)	4.8E2 (R,D)	—	7.9E3 (R,P)	1.4E2	R
	21A	2-methylnaphthalene	2.1E3 (R,P)	2.2E2 (R,D)	—	1.0E4 (R,P)	3.3E2	R
	21A	C_2-alkylnaphthalene	1.5E5 (C,D)	—	—	1.6E4 (R,P)	5.0E2	C
+	21A	anthracene	1.9E4 (C,D)	4.1E1 (R,D)	—	2.3E4 (R,P)	6.9E2	R
	21A	C_2-alkylanthracene	—	—	—	2.1E3 (C,P)	8.0E1	C
	21A	9-methylanthracene	4.6E4 (C,D)	—	—	1.6E4 (R,P)	—	
+o	21A	phenanthrene	1.9E4 (C,D)1/1	9.6E1 (R,D)	1.0E-1 (G,D)	2.3E4 (R,P)0/-	7.6E2	R
+o	21A	acenaphthene	4.1E4 (C,D)1/Y	—	—	4.2E3 (R,P)	1.5E2	C
+o	21A	acenaphthylene	2.8E4 (C,D)1/1	4.1E3 (C,S)	—	1.8E4 (R,P)0/0	4.3E2	C
o	21A	C_2-alkylacenaphthalene	3.3E3 (C,D)0/0	—	—	—	—	
o	21A	C_2-alkylacenaphthene	3.5E3 (C,D)0/0	—	—	1.2E3 (C,P)	1.2E2	C
	21A	C_3-alkylacenaphthene	—	—	—	5.0E2 (C,P)	5.1E1	C
o	21A	binaphthyl	1.4E4 (C,P)1/1	—	—	—	2.8E-1	C
o	21A	methylacenaphthylene	1.3E4 (C,D)1/1	—	—	2.8E3 (C,P)	2.8E2	C
o	21A	methylacenaphthene	1.6E4 (C,D)1/1	—	—	6.0E2 (C,P)	6.3E1	C
	21A	9-methylanthracene	—	—	—	—	5.3E2	R
	21A	$C_{15}H_{12}$:3 rings	8.0E1 (R,P)	—	—	—	2.0E-1	R
+o	21B	benzo(a)anthracene	1.8E3 (F,P)1/1	—	—	7.0E3 (R,P)2/2	1.6E2	R
o	21B	7,12-dimethylbenzo(a)-anthracene	1.3E5 (F,P)-/6	—	—	—	3.3E-1	FS
o	21B	methylphenanthracene	—	—	—	2.1E3 (C,P)3/3	2.1E2	C
o	21B	methyltriphenylene	—	—	—	1.2E3 (C,P)3/3	1.2E2	C

Table 1. *(Continued)*

	MEG Category	Chemical Name	Maximum Concentration (Source, Stream Type) $log_{10}DS_n/log_{10}DS_e$ Gas (µg/m³)	Liquid (µg/l)	Solid (µg/g)	Tar (µg/g)	Maximum Production Factor & Source µg/g coal	
o	21B	triphenylene	—	5.0E1 (R,D)1/1	—	6.2E3 (R,P)4/4	2.9E2	C
o	21B	$C_{18}H_{10}$:4 rings	1.7E2 (R,P)3/3	—	—	—	4.3E-1	R
o	21B	3-methylcholanthrene	4.7E0 (F,P)0/0	—	—	—	9.6E-3	FS
o	21B	benzo(c)phenanthrene	1.0E3 (F,P)0/0	—	—	—	2.0E0	FS
+o	21B	chrysene	7.3E3 (C,D)0/1	1.6E2 R,D)	—	8.6E3 (R,P)0/0	2.9E2	C
	21B	methyl chrysene	—	—	—	1.2E3 (C,P)	5.4E2	C
+	21B	pyrene	9.2E3 (C,D)	—	—	2.4E4 (R,P)	7.2E2	R
	21B	1-methylpyrene	—	—	—	3.8E3 (C,P)	3.8E2	C
+o	21C	dibenzo(a,h)anthracene	6.1E0 (F,P)2/2	—	—	3.4E3 (R,P)4/4	9.3E1	R
+o	21C	benzo(a)pyrene	5.0E3 (C,D)5/6	3.6E1 (R,D)2/2	—	3.5E3 (R,P)5/5	1.2E2	R
o	21C	perylene	4.9E3 (C,D)5/5	2.1E1 (R,D)2/2	—	3.7E3 (R,P)5/5	8.0E1	C
	21C	benzo(e)pyrene	—	2.1E1 (R,D)	—	2.1E3 (R,P)	6.9E1	R
o	21D	benzoperylene	1.6E3 (C,D)1/1	3.4E4 (C,S)2/2	—	— 1/1	5.0E1	C
+	21D	benzo(g,h,i)perylene	—	—	—	2.7E3 (R,P)	4.8E1	R
	22A	C_2-alkylindene	3.8E4 (C,D)	—	—	3.0E2 (C,P)	3.7E1	C
	22A	C_3-alkylindene	8.0E3 (C,D)	—	—	—	1.4E0	C
+	22A	fluorene	9.1E3 (C,D)	5.7E1 (R,D)	1.0E1 (G,D)	8.0E3 (R,P)	2.6E2	R
o	22A	methylindene	8.4E4 (C,D)0/0	3.4E3 (C,S)	—	—	1.5E1	C
	22A	methylfluorene	4.1E3 (C,D)	—	—	2.1E3 (C,P)	—	
+o	22B	benzofluorene (fluoranthene)	9.2E3 (C,D)	2.8E1 (R,D)	—	3.4E4 (R,P)1/-	3.8E2	C R
	22B	fluoranthene	—	—	—	—	1.0E3	R
	22B	benzo(b)fluorene	—	—	—	3.8E3 (C,P)	5.6E1	R
	22B	benzo(a)fluorene	—	—	—	4.1E3 (R,P)	8.6E1	R
+	22C	benzo(k)fluoranthene	—	1.7E1 (R,P)	—	1.6E3 (R,P)	—	
	22C	benzo(h)fluoranthene	—	—	—	—	5.3E1	R
	22C	benzo(b)fluoranthene	3.8E2 (F,P)	3.3E1 (R,D)	—	3.2E3 (R,P)	1.0E2	R
+	22D	indeno(1,2,3-cd)pyrene	—	—	—	1.7E3 (R,P)	4.6E1	R
	23A	pyridine	9.2E2 (C,D)	2.8E4 (K,S)	—	—	1.6E-1	C
o	23A	C_2-alkylpyridine	1.6E4 (C,D)-/0	2.6E4 (K,S)	—	—	2.8E0	C
	23A	C_3-alkylpyridine	1.0E4 (C,D)	1.0E3 (C,S)	—	1.0E2 (C,P)	1.2E1	C
	23A	C_4-alkylpyridine	—	—	—	2.0E2 (C,P)	2.0E1	C
	23A	methylpyridine (picolines)	4.0E3 (C,D)	—	—	—	7.1E-1	C
	23A	2-methylpyridine	—	—	—	—	2.5E1	K
	23A	3-methylpyridine	—	—	—	—	1.1E1	K
	23A	4-methylpyridine	—	—	—	—	1.1E1	K
o	23A	dimethylpyridine	—	4.6E4 (K,S)-/0	—	—	—	
	23A	2-methylpyridine	—	2.9E4 (K,S)	—	—	—	
	23A	3,4-methylpyridine	—	1.3E4 (K,S)	—	—	—	
	23B	quinolines	4.8E3 (C,D)	5.0E3 (K,S)	—	1.9E4 (C,P)	1.9E3	C
	23B	C_2-alkylquinolines	5.4E3 (C,D)	1.2E4 (K,S)	—	2.3E3 (C,P)	2.3E2	C
	23B	C_3-alkylquinolines	4.6E2 (C,D)	—	—	1.1E3 (C,P)	1.1E2	C
	23B	2-methylquinoline	3.5E3 (C,D)	1.8E3 (C,S)	—	6.0E2 (C,P)	6.0E1	C
	23B	acridine	8.4E3 (C,D)	—	—	1.7E3 (R,P)	9.0E1	C
	23B	C_3-alkylacridine	—	—	—	6.0E2 (C,P)	6.0E1	C
	23B	C_2-alkylacridine	—	—	—	9.0E2 (C,P)	9.0E1	C
	23B	C_2-alkylbenzoquinoline	—	—	—	3.0E3 (C,P)	—	
	23B	C_3-alkylbenzoquinoline	—	—	—	6.0E2 (C,P)	6.0E1	C
	23B	methylacridine	4.8E3 (C,D)	—	—	4.0E2 (C,P)	4.0E1	C
	23B	dihydroacridine	1.1E1 (F,P)	—	—	—	2.2E-1	FS
o	23B	methylbenzophenanthridine	2.4E3 (C,D)-/1	—	—	—	4.8E-2	C
	23B	benzophenanthridine	4.8E3 (C,D)	—	—	—	9.6E-2	C
	23B	benzoquinoline (phenanthridine)	—	—	—	7.0E2 (C,P)	7.0E1	C
	23B	methylbenzoquinoline	—	—	—	1.1E3 (C,P)	3.0E2	C
	23C	indole	—	5.3E4 (C,S)	—	5.8E1 (R,P)	1.9E0	R
	23C	methylindole	—	8.9E3 (C,S)	—	—	—	
o	23C	carbazole	4.9E3 (C,D)	—	—	2.7E3 (R,P)1/-	5.3E1	R
	23C	methylcarbazole	—	—	—	2.0E2 (C,P)	2.0E1	C
o	23C	pyrroline**	2.0E3 (C,D)1/1	—	—	—	4.0E-2	C
	24A	methyldioxolane	—	5.0E0 (C,S)	—	—	—	
	24A	benzofuran	5.5E4 (R,P)	—	—	—	1.3E2	R
	24A	dibenzofuran	1.2E4 (R,P)	—	—	8.1E3 (R,P)	2.7E2	R
o	25A	thiophene	2.3E6 (R,P)3/3	—	—	—	3.7E3	R

Table 1. *(Continued)*

	MEG Category	Chemical Name	Maximum Concentration (Source, Stream Type) $\log_{10}DS_n/\log_{10}DS_e$ Gas (µg/m³)	Liquid (µg/l)	Solid (µg/g)	Tar (µg/g)	Maximum Production Factor & Source µg/g coal
o	25A	C_2-thiophenes	7.8E4 (R,P)1/1	—	—	—	3.3E2 R
o	25A	methylthiophene	8.7E4 (R,P)0/0	—	—	—	2.9E2 R
	25A	dimethylthiophene	1.5E4 (R,P)	—	—	—	5.0E1 R
	25B	benzothiophene	—	—	—	8.7E3 (R,P)	2.6E2 R
o	27	lithium	4.3E3 (F,P)2/2	4.0E2 (F,D)0/0 (G/D)	2.4E2 (G,D)0/0	—	4.1E1 FS
o	28	sodium	2.1E4 (F,P)	1.7E6 (F,D)1/1	1.8E4 (F,D)	—	1.5E4 FS
o	29	potassium	1.0E4 (C,D)1/1	2.0E4 (C,S)	4.0E5 (C,D)	3.0E3 (C,P)	7.3E3 FS
	30	rubidium	1.0E1 (C,D)	2.0E2 (G,D)	2.0E4 (C,D)	5.0E-1 (C,P)	1.2E3 C
	31	cesium	2.3E1 (F,P)	4.0E0 (F,D)	1.5E1 (G,D)	—	6.8E0 FS
+o	32	beryllium	2.6E0 (F,P)0/0	1.0E0 (G,D) (K,S)	2.7E1 (R,D)1/1	—	7.6E0 FS
o	33	magnesium	3.9E4 (F,P)1/1	1.1E4 (F,D)	1.3E4 (F,D)	2.0E2 (C,P)	1.1E4 FS
	33	rhenium	3.0E-1 (F,P)	—	1.0E-1 (G,D)	—	6.1E-1 FS
o	34	calcium	1.5E5 (F,P)-/1	2.2E5 (F,D)	5.0E4 (F,D)0/0	—	4.4E4 FS
o	35	strontium	3.9E3 (F,P)0/0	4.0E3 (F,D)	2.0E3 (C,D)	2.0E1 (C,P)	1.6E3 FS
o	36	barium	7.5E3 (F,P)1/1	1.0E4 (G,D)0/0	5.5E3 (F,D)1/1	5.0E1 (C,P)	4.7E3 FS
	37	boron	5.6E2 (F,P)	9.0E3 (C,S)-/1	2.1E2 (F,D)	1.0E0 (C,P)	1.8E2 FS
o	38	aluminum	2.7E4 (F,P)-/0	1.1E4 (F,D)	8.8E4 (F,D)-/1	—	7.5E4 FS
	39	gallium	9.0E1 (C,D)	4.0E1 (G,D)	2.2E2 (G,D)	9.0E0 (C,P)	8.0E0 FS
+	41	thallium	1.0E1 (C,D)	4.0E0 (K,S)	2.2E1 (G,D)	—	4.8E-2 GG
o	42	carbonate	2.0E0 (C,P)	2.0E6 (C,S)1/1	—	—	3.5E-4 C
o	42	carbon dioxide	1.8E9 (K,D)2/2	—	—	—	1.2E6 R
o	42	carbon monoxide	3.0E8 (R,P)4/4	—	—	—	9.8E5 R
o	43	silicon	8.0E3 (C,D)	1.0E4 (G,D)	1.4E5 (F,D)0/0	—	4.3E2 C
	44	germanium	7.2E0 (F,P)	3.0E1 (K,S)	1.1E1 (G,D)	—	1.1E-1 FS
	45	tin	8.0E0 (C,D)	3.0E3 (F,D)	3.0E2 (C,D)	—	1.8E1 C
+o	46	lead	1.7E2 (F,P)0/0	4.5E2 (F,D)-/0 (G,D)	2.3E2 (G,D)0/0	5.0E1 (C,P)0/0	1.1E1 R
+o	47	ammonia	3.2E8 (K,D)4/4	7.9E6 (R,D)3/3	—	—	8.8E3 R
+o	47	cyanide	5.0E4 (C,D)1/1	1.0E6 (R,D)3/5 (C,S)	—	—	2.1E1 R
o	47	hydrogen cyanide	5.8E6 (K,D)-/3	8.6E3 (R,P)-/1	—	—	9.42 K
	47	nitrate	—	1.7E4 (G,D)	—	—	9.7E0 K
	47	nitrite	—	1.0E1 (F,D)	—	—	5.0E-4 FS
o	47	nitrogen dioxide	3.0E5 (C,D)1/1	—	—	—	5.3E1 C
o	47	nitorgen oxide	4.0E4 (C,D)0/0	—	—	—	7.3E0 C
o	48	phosphorus	3.3E3 (F,P)1/1	2.0E4 (C,S)0/0	8.0E3 (C,D)0/0	—	1.7E3 FS
	48	phosphate	—	2.5E3 (K,S)	2.0E3 (F,D)	—	9.6E1 GG
+o	49	arsenic	4.0E2 (F,P)2/2	1.8E3 (R,D)3/2	8.5E1 (G,D)2/0	4.4E0 (R51,P)1/-	2.7E1 GS
+o	50	antimony	4.0E2 (F,P)	2.0E2 (R,D)	2.0E2 (C,D)0/0	8.0E1 (C,P)	1.3E1 C
	51	bismuth	2.6E0 (F,P)	—	1.8E1 (G,D)	5.0E0 (C,P)	1.7E0 GG
o	53	sulfur	1.0E4 (C,D)	9.7E5 (F,D)0/0	1.5E4 (G,D)	1.8E4 (R21,P)	7.6E3 FS
o	53	carbon disulfide	8.4E4 (R,P)1/1	—	—	—	2.8E2 R
o	53	carbonyl sulfide	1.1E6 (K,S)2/2	—	—	—	1.3E3 R
o	53	hydrogen sulfide	6.9E7 (K,S)3/3	—	—	—	4.1E4 R
o	53	sulfate	5.0E3 (C,D)1/1	2.8E6 (F,D)-/1	—	—	9.7E1 K
o	53	sulfide	2.0E5 (C,D)2/1	1.0E4 (C,S)1/3	—	—	—
	53	sulfite	—	4.7E4 (F,D)0/0	—	—	1.2E0 FS
o	53	sulfur dioxide	6.9E4 (G,D)0/0	—	—	—	1.7E0 C
o	53	thiocyanate	1.0E5 (C,D)1/1	2.7E5 (K,S)3/1 (R,D)	—	—	5.9E2 R
+o	54	selenium	1.5E4 (F,P)2/2	2.0E3 (C,S)1/2	5.8E1 (R,D)1/1	2.7E0 (R51,P)	4.4E1 FS
	55	tellurium	9.7E-1 (F,P)	—	9.0E-1 (G,D)	—	2.0E-2 GG
o	56	fluorine (fluoride)	1.3E3 (F,P)	2.0E5 (C,S)1/1	2.8E2 (F,D)	2.0E1 (C,P)	1.7E2 FS
			—	—	—	—	5.9E0 GG
o	57	chlorine (chloride)	3.0E4 (C,D)1/1	8.6E6 (R,D)1/1	1.5E2 (F,D)	—	4.8E3 R
			—	—	—	—	2.8E3 R
	58	bromine (bromide)	1.3E2 (F,P)	1.3E4 (R,D)	9.7E1 (R,D)	1.2E0 (R50,P)	2.9E1 GG
			—	—	—	—	5.8E-1 C
	59	iodine (iodine)	4.0E0 (F,P)	4.0E2 (K,S)	2.4E1 (G,D)	5.0E0 (C,P)	5.0E1 GG
			—	—	—	—	5.0E-2 R
	60	scandium	1.9E1 (F,P)	7.0E0 (G,D)	5.0E1 (C,D)	1.0E0 (C,P)	3.5E0 FS

Table 1. (Continued)

	MEG Category	Chemical Name	Maximum Concentration (Source, Stream Type) $\log_{10}DS_n/\log_{10}DS_s$ Gas (µg/m³)	Liquid (µg/l)	Solid (µg/g)	Tar (µg/g)	Maximum Production Factor & Source µg/g coal	
	61	yttrium	3.0E1 (F,P)	4.0E1 (G,D)	5.9E1 (F,D)	1.0E0 (C,P)	5.0E1	FS
	62	titanium	1.0E3 (C,D)	1.0E4 (G,D)	4.5E3 (F,D)	—	3.8E3	FS
	63	zirconium	1.0E3 (C,P)	2.0E2 (G,D)	3.5E2 (G,D)	—	1.5E2	FS
	64	hafnium	2.9E0 (F,P)	—	3.0E0 (G,D)	—	8.6E-1	FS
	65	vanadium	1.0E2 (C,D)	5.0E2 (G,D)	4.1E2 (F,D)	1.0E0 (C,P)	3.5E2	FS
	66	niobium	4.0E2 (C,D)	3.0E1 (G,D)	5.2E1 (G,D)	5.0E0 (C,P)	2.6E1	FS
+o	68	chromium	8.0E2 (C,D)3/3	2.4E3 (R,D)3/1	3.4E3 (R,D)4/5	1.9E2 (R,P)3/4	5.5E2	C
	69	molybdenum	4.0E2 (C,D)	4.0E2 (G,D)	5.7E1 (G,D)	—	1.4E1	GG
	70	tungsten	4.0E0 (C,D)	2.0E1 (F,D;	5.0E0 (G,D)	—	8.7E-1	FS
+	71	manganese	1.9E2 (R,P)	4.0E1 (K,S)	5.7E2 (G,D)	6.8E-1 (R,P)	1.9E2	FS
o	72	iron	3.3E4 (F,P)1/1	5.0E3 (G,D)0/0	9.0E4 (F,D)2/2	2.3E-2 (R,P)	7.6E4	FS
o	72	iron carbonyls***	1.3E5 (G,D)2/2	—	—	—	1.1E0	GG
	74	cobalt	1.5E1 (F,P)	4.0E1 (G,D)	5.0E1 (C,D)	1.1E-1 (R,P)	2.0E1	FS
+o	76	nickel	1.2E2 (F,P)1/1	8.0E1 (K,S)	3.7E2 (R,P)1/1	5.0E0 (R,P)	6.4E1	FS
	76	nickel carbonyl***	2.9E1 (G,D)	—	—	—	2.0E-4	GG
+o	73	copper	2.0E3 (C,D)1/1	4.9E2 (R,D)-/2	1.0E3 (C,D)0/0	3.0E3 (C,P)0/0	1.0E2	C
+o	79	silver	1.0E3 (C,D)2/2	2.0E0 (G,D) (C,S) (F,D)-/1	5.0E0 (G,D)	—	8.1E-1	FS
	80	gold	—	—	1.0E0 (G,D)	—	8.6E-4	GG
+	81	zinc	1.0E3 (C,D)	5.4E2 (R,D)	1.0E3 (G,D)	1.9E1 (R,P)	2.0E1	FS
+o	82	cadmium	2.7E2 (F,P)1/1	5.0E0 (C,S) (F,D)-/C	9.0E0 (C,D)-/1	1.4E0 (R,P)-/1	6.9E1	FS
+o	83	mercury	6.5E3 (F,P)2/2	6.3E2 (K,S)3/3	2.8E2 (G,D)3/3	6.0E-2 (C,P)	1.4E1	FS
	84	cerium	6.0E1 (C,P)	1.0E2 (G,D)	1.8E2 (G,D)	5.0E0 (C,P)	9.3E1	FS
	84	dysprosium	1.7E0 (F,P)	3.0E0 (G,D)	3.0E0 (G,D)	—	1.2E-2	FS
	84	erbium	6.4E-1 (F,P)	1.0E0 (G,D)	1.0E0 (G,D)	—	1.3E-3	FS
	84	europium	9.7E-1 (F,P)	1.0E0 (G,P)	1.0E0 (G,D)	—	2.0E-3	FS
	84	gadolinium	1.9E0 (F,P)	2.0E0 (G,D;	2.0E0 (G,D)	—	3.9E-3	FS
	84	holmium	9.7E-1 (F,P)	2.0E0 (G,D)	2.0E0 (G,D)	—	2.0E-3	FS
	84	lanthanum	1.0E2 (C,D)	5.0E1 (G,D)	1.6E2 (G,D)	5.0E0 (C,P)	9.3E1	FS
	84	lutetium	—	1.0E0 (G,D)	3.0E-1 (G,D)	—	2.9E-2	GG
	84	neodymium	9.7E0 (F,P)	1.0E1 (G,D)	1.1E2 (G,D)	—	2.5E1	FS
	84	praseodymium	6.4E0 (F,P)	1.0E1 (G,D)	3.5E1 (G,D)	—	1.4E1	FS
	84	samarium	6.4E0 (F,P)	1.0E1 (G,D)	1.3E1 (F,D)	—	1.1E1	FS
	84	terbium	6.4E-1 (F,P)	1.0E0 (G,D)	6.0E-1 (G,D)	—	6.8E-2	GG
	84	thulium	<3.0E-1 (F,P)	1.0E0 (G,D)	2.0E-1 (G,D)	—	1.9E-2	GG
	84	ytterbium	—	2.0E0 (G,D)	2.0E0 (G,D)	—	1.9E-1	GG
	85	thorium	1.0E1 (C,D)	4.0E1 (G,D)	9.8E1 (R,D)	—	2.0E1	FS
o	85	uranium	7.0E3 (C,D)3/3	4.0E1 (K,S)	4.0E2 (C,D)	—	1.4E1	FS
o	99	hydrogen	5.4E7 (K,S)2/2	—	—	—	4.0E4	K

+Priority pollutant
oDischarge severity exceeds 1
**Probable artifact
***Inferred concentration
- no DMEG value available

Source gasifier
G = Wellman-Galusha (Glen-Gery)
F = Wellman-Galusha (Ft. Snelling)
C = Chapman
R = RTI Run
K = Kosovo Lurgi

Source stream classification
D = Discharge
P = Product or by-product
S = Process stream

qualitatively identified (in approximately 70 experimental gasification tests at RTI's fossil energy laboratories) but not quantitated. MEG numbers refer to the ordering system of chemical categories found in the MEG reports.

Results and Conclusions

In addition to Table 1, Figures 1 through 9 summarize results from data analysis. Of the 276 compounds and elements quantitated in Table 1, 128 have discharge severities greater than 1 (potential hazard) in one stream or another. Of the species quantitated in Table 1, 39 are priority pollutants;[17] of these, 30 were detected at potentially hazardous levels, $DS < 1$.

Table 2. Additional Substances Identified in RTI Coal Gasification Effluent Streams

MEG No.	Compound
01A	n-pentane
01A	isopentane
01A	cyclopentane
01A	n-hexane
01A	isohexane
01A	cyclohexane
01A	n-heptane
01A	n-octane
01A	n-nonane
01A	n-decane
01A	n-undecane
01A	n-dodecane
01A	dimethylcyclohexane
01A	trimethylcyclohexane
01A	dimethyldecahydronaphthalene
01A	3-methylpentane
01A	methylcyclobutane
01A	n-hexadecane
01B	1-butene
01B	3-methyl-1-butene
01B	pentadiene
01B	methylisopropanone
01C	acetylene
01C	propyne
02A	methylene chloride
02A	chloroform
03A	diethylether
03A	phenyl-2-propynylether
03A	3,6-dimethoxphenanthrene
05A	3,5,5-trimethyl-1-hexanol
07A	acetaldehyde
07A	butyraldehyde
07A	benzaldehyde
07A	dimethylbenzaldehyde
07A	n-nonanal
07A	phenanal
07A	n-octanal
07A	undecanal
07A	dodecanal
07B	acetone
07B	butanone
07B	acetophenone
07B	dihydroxyanthraquinone
07B	benzophenone
07B	1-phenyl-1-propanonephthalate
07B	2-pentanone
07B	o-hydroxyacetophenone
07B	m-hydroxyacetophenone
07B	tetrahydroanthraquinone
07B	dihydroxyanthraquinone
07B	methylisopropyl ketone
08A	acetic acid
08A	benzoic acid
08A	1,4-benzenedicarboxaldehyde
08C	benzamine
08C	diethyl phthalate
08D	ethyl acetate
08D	methyl benzoate
08D	ethylbenzyl acetate
08D	isobutylcinnamate
08D	dibutyl phthalate
08D	diisobutyl phthalate
08D	dicyclohexyl phthalate
08D	p-tert-butylphenoxymethyl-acetate
08D	butylphthayl glycolate
08D	di-2-ethylhexyl phthalate
08D	butylphthalylbutylphthalate
08D	di-n-octylphthalate
08D	di-2-ethylhexyl phthalate
09A	acetonitrile
09B	benzonitrile
09B	2,2-dicyanobiphenyl
09B	cyanobutadiene
10C	aniline
10C	aminotoluenes
10C	benzidine
10C	2-aminonapthalene
10C	n-methyl-o-toluidine
13A	benzenethiol
13A	toluenethiol
13B	2,3,4-trithiapentane
13B	dimethyl disulfide
13B	trithiahexane
13B	diphenyl disulfide
15A	diphenylethyne
15A	isopropylbenzene
15A	1,2-diphenylpropane
15A	methylphenylethyne
15A	dixylylethane
15A	phenylbenzaldehyde
15A	propylbenzene
15B	o-diethylbenzene
15B	m-diethylbenzene
15B	p-diethylbenzene
15B	o-terphenyl
15B	m-terphenyl
15B	p-terphenyl
15B	1,2,3-trimethylbenzene
15B	1,2,4-trimethylbenzene
15B	1,3,5-trimethylbenzene
15B	methylindene
15B	methylbiphenyl
15B	dimethylindan
15B	methyltetrahydronaphthalene
15B	3,5-dimethyl-1-isopropyl-benzene
15B	5,8-dimethyl-1-n-octyl-1,2,3,4-tetrahydronaphthalene
15B	1-methyl-4-n-heptinyl-1,2,3,4-tetrahydronaphthalene
15B	dimethyltetrahydronaphthalene
15B	dimethylindene
15B	trimethylindene
15B	pentamethylindan
15B	3-methylbiphenyl
15B	ethylstyrene
15B	methylstyrene
15B	1,2-dimethylethylbenzene
15B	methyl-2,3-dihydroindene
15B	n-pentylbenzene
15B	trimethyltetrahydrophthalene
17B	2-nitrodimethyl-1,4-benzene-dicarboxylate
17B	1-nitroso-2-hydroxynaphthalene
18A	m-cresol
18A	p-cresol
18A	2,3-xylenol
18A	2,4-xylenol
18A	2,5-xylenol
18A	2,6-xylenol
18A	3,5-xylenon
18A	3,4-xylenol
18A	alkyl cresols
18A	6-ethyl-m-cresol
18A	hydroxyisopropylbenzene
18A	4-tert-butyl-o-cresol
18A	1-allyphenol
18A	di-t-butyl-4-ethylphenol
18C	2-naphthol
18C	2-hydroxyfluorene
18C	2-methoxyfluorene
18C	phenanthridone
18C	methylhydroxynaphthalene
21A	1-ethylnaphthalene
21A	dimethylnaphthalenes
21A	1,4-diemthylnaphthalene
21A	2,3-dimethylnaphthalene
21A	2,6-dimethylnaphthalene
21A	methyldihydronaphthalene
21A	cyclobutadibenzene
21A	propenylphenanthrene
21A	9-methylanthracene
21A	isopropylnaphthalene
21A	4,5-methylenephenanthrene
21A	2,7-dimethylphenanthrene
21A	1-methylphenanthrene
21A	2-methylphenanthrene
21A	2-benzylnaphthalene
21A	trimethylnaphthalene
21A	trans-9-propenylphenanthrene
21A	2-methoxynaphthalene
21A	1-methoxynaphthalene
21A	1,2-dihydro-3,5,8-trimethyl naphthalene
21A	1-methyl-7-isopropylnaphthalene
21A	8-n-butylphenanthrene
21A	ethylanthracene
21A	3-methylacenaphthalene
21A	methylacenaphthalene
21B	naphthacene
21B	benzo(a)anthracene
21B	benzo(c)phenanthrene
21B	1-methylbenzo(c)phenanthrene
21B	methyl chrysenoid
21B	1-methylpyrene
21B	methylbenz(a)anthracene

Table 2. (Continued)

MEG No.	Compound	MEG No.	Compound	MEG No.	Compound
21B	1,2,3,4-tetrohydro-9,10-benzophenanthrene	23B	azapyrene	24A	7-methylbenzofuran
		23B	benzacridines	24A	dimethylbenzofuran
21B	hexhydrobenz(a)anthracene	23B	6-methylquinoline	24A	dihydromethylphenylbenzofuran
21B	2-methyl-9,10-benzophenanthrene	23B	3-methylquinoline	24A	3,3-dihydro-2-methylbenzofuran
		23B	8-n-propylquinoline	24A	3,6-dimethylbenzofuran
21B	methylbenzo(a)anthracene	23B	ethylquinolines	24B	xanthene
21B	5,8-dimethylbenz(c)phenanthrene	23B	3-n-propylquinoline	25A	2-methylthiophene
		23B	4-n-propylquinoline	25A	3-methylthiophene
21C	perylene	23B	3-methylbenzoquinoline	25A	2,3-dimethylthiophene
21C	2-n-hexylperylene	23B	4-styryloquinoline	25A	2,4-dimethylthiophene
22A	1-methylfluorene	23B	methylphenylquinoxaline	25A	2,5-dimethylthiophene
22A	9-fluorenone	23C	pyrrole	25A	3,4-dimethylthiophene
22A	methylfluorene	23C	phenylindole	25A	trimethyl and tetramethyl thiophene
22A	dimethylfluorene	23C	benzothiazole	25A	isopropylthiophene
22B	1,2-benzofluorene	23C	vinylphenylcarbazole	25A	ethylthiophene
22B	1,2,3,4-tetrahydrofluoranthrene	23C	1,2,3,4-tetrahydrocarbazone	25A	2-n-propyl-5-isobutylthiophene
				25B	benzo(b)thiophene
22B	benzofluorenone	23C	methyl-3-allylhydroindole	25B	dibenzothiophenes
23A	collidines	23C	3-methyl-3-allyldihydrindole	25B	dihydrobenzothiophene
23A	2,4-dimethyl-6-ethylpyridene			25B	methylbenzothiophenes
		23C	3-amino-9-ethylcarbazole	25B	phenanthro(4,5-bcd)thiophene
23A	4-acetylpyridine	23C	3-methyl-2-phenylindole	25B	naphthothiophenes
23A	2-hydroxy-4-phenylpyridine	23C	3-benzylindene phthalimide	25B	dianphthothiophenes
23A	2-hydroxy-6-phenylpyridine	23C	1,4-dihydro-2,3-benzo(b) carbazole	25B	methyldibenzothiophenes
23A	2,2-dimethyl-4,4-dipyridyl			25B	trimethylbenzothiophene
23A	3,4-diphenylpyridine	23C	3,3-bliniolyl	25B	methylbenzothiophene
23B	isoquinoline	23D	2-ethylbenzimidazole	25B	benzodithiophene
23B	phenylpyridine	23D	diphenyldiazole	25B	1,3-dihydro-4,6-dimethyl thieno(3,4-C)thiophene
23B	azobenzene	23D	methylbenzimidazol		
23B	7,8-benzoquinoline	23D	2-methyl-5-phenyltetrazole	25B	1-methylbenzo(1,2-B14,3) dithiophene
23B	5,6-benzoquinoline	23D	2-amino-5-chloro-4,6-dimethylpyrimidine		
23B	2,6-dimethylquinoline			25B	3-methyldibenzothiophene
23B	benzo(h)quionline	23D	2-amino-4-phenyl-6-methyl pyrimioine	25B	5-methyl-2,3-benzothiophene
23B	ethylquinoline			25B	methylbenzothiophene
23B	3-methylbenzoquinoline	23D	4-(1,2,3,4-tetrahydro-2-naphthyl)-moropholine	25B	2,6-dimethylbenzc(b)thiophene
23B	dimethylacridine			26A	tributyl phosphate
23B	azafluoranthene	23D	2-benzimilizole	53A	ethyl isothiocyanate

The following emphasizes only those substances possessing singularly high levels of Discharge Severity (DS), Control Priority (CP), and/or Production Factor (PF). Pollutants were selected first on the basis of health, rather than ecological DMEG. Two other criteria were applied to selecting compounds for representation in the figures: 1) where a class of compounds (e.g., two- and three-ring fused polycyclic hydrocarbons - MEG category 21A) is well represented by the analytical data and CP or DS do not vary greatly within the class, preference is given to those compounds for which chemical analytical identification confidence is highest and/or which represent high production levels (PF); and 2) within classes of compounds, preference is given to those compounds for which a specific DMEG has been derived (i.e., those not assigned a DMEG by class association only). These criteria compensate for the inherent inaccuracies in DMEG estimations, and also demonstrate some important potential candidates for elimination from consideration as environmental hazards.

In Figure 1, 28 pollutants (from all streams and sources investigated) are estimated to be of first priority concern. These are ranked in descending order of CP. Fused polycyclic hydrocarbons and phenols lead the list. The PF and DS values listed show that many of the most potentially hazardous substances receive a high rank because of a low DMEG, rather than high production. Where PF values approach or lie to the right of CP values, higher level of production is an important consideration in hazard potential; e.g., for Fe, NH_3, and H_2S. Where DS_n values approach or lie to the right of CP values, maximum stream concentration is high (e.g., for cresols, perylene, benzene, and ammonia), and it is likely that the stream represented by the maximum concentration is responsible for a high percentage of the total production of that pollutant. Obviously where PF, CP, and DS are all high, the pollutant and stream must be given first consideration for environmental control. Such substances as iron and chromium may be produced from reactor or other materials corrosion, rather than from the coal gasification.

Figure 2 lists the same compounds as in Figure 1, but evaluation is based on ecological DMEGs, rather than health hazard. When ecological effects are considered, potential hazard is increased for chromium, benzo(a)pyrene, benzene, mercury, cadmium, and selenium (in

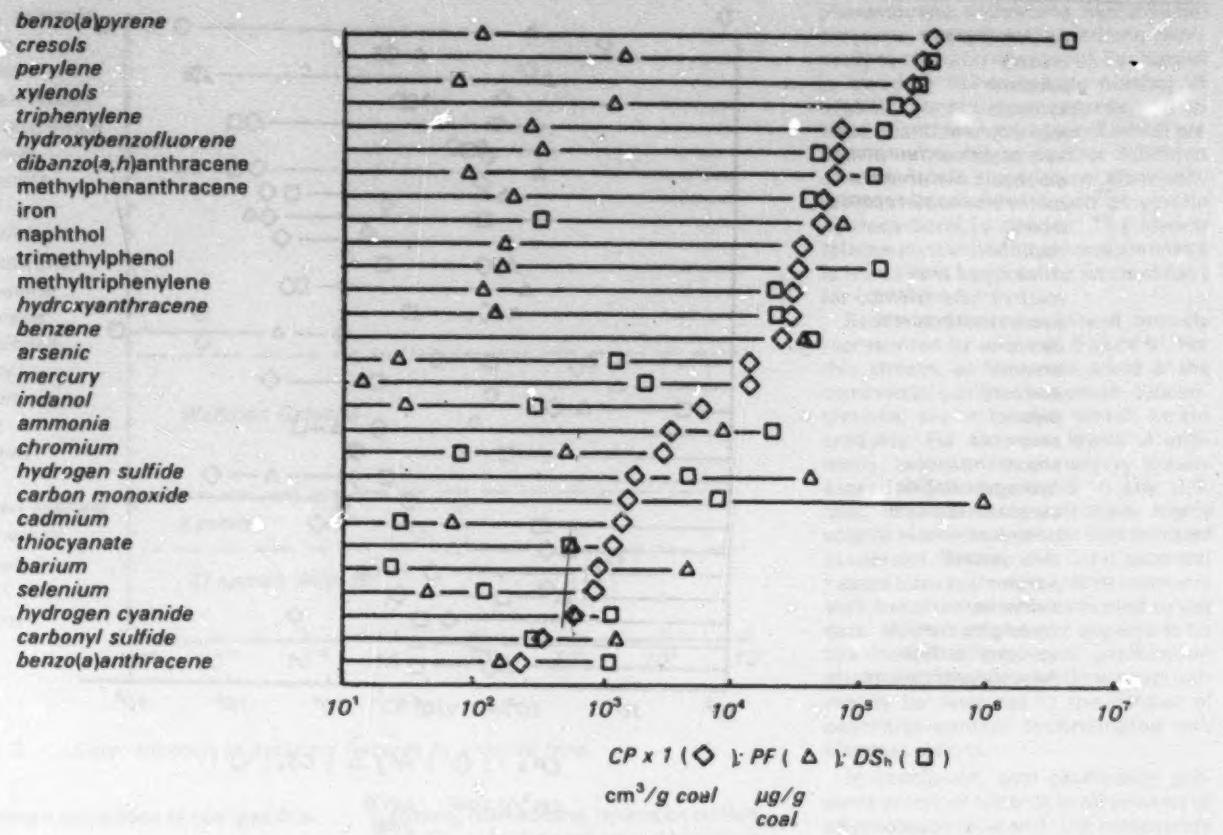

Figure 1. Health hazard indices and production levels for potentially hazardous coal gasification pollutants.

terms of increased DS value). Ecological CP values are higher for mercury, hydrogen sulfide, cadmium, and selenium. Ecological DMEGs are often reduced for metals below the DMEGs for health, primarily because cytotoxicity studies are available which recommend stringent controls.

Noted in Table 1 that, while a preponderence of quantitations are associated with commercial gasifiers, many of the concentrations are at nonhazardous levels, and indeed lie within the realm of extremely difficult analytical identification. Figure 3 illustrates the most potentially hazardous compounds (on the basis of CP) which were sampled and quantitated for all the processes considered. These substances are quite important because of their consistent presence under a wide range of gasification system conditions. RTI's experimental program has involved selection and emphasis of the worst and most prevalent pollutants from coal gasification, and observation of production under a broad range of operating conditions and coal types. This accounts for most of the bias in data toward the RTI system. Of the substances found in Figures 1 and 2, 13 are missing in Figure 3 because they were not always analyzed: benzo(a) pyrene, perylene, triphenylene, hydroxybenzofluorene, dibenzo(h)anthracene, methylanthracene, iron, trimethylphenol, methyltriphenylene, hydroxyanthracene, arsenic, indenol, and benzo(a)anthracene. All the maximum concentrations for the two Wellman-Galusha gasifiers are for inorganics.

Figure 4 shows the distribution of significant pollutants by stream characterization. As stated earlier, streams are best characterized by discharge severity, DS, and CP comparison is preferred for processes. The most important result demonstrated is that most of the potentially hazardous pollutants are found in product/byproduct and discharge streams with a high potential for leaving the plant boundaries and possibly of contaminating the environment. Ranking on the basis of discharge severity also makes some changes in the pollutants selected, since some pollutants with low production levels may have high stream concentrations. Hazardous substances shown in Figures 1 and 2 (but not in Figure 4) include iron, arsenic, indanol, cadmium, thiocyanate, beryllium, selenium, hydrogen cyanide, carbonyl sulfide, and benzo(a)anthracene (the last seven are at the bottom of the CP ranking list). Compounds added on the basis of the DS value include 7,12-dimenthylbenzo(a)anthracene, cyanide, uranium, isopropylphenol, C_2-alkylphenol, C_2-alkylhydroxypyrene, C_5-alkylhydroxyanthracene, C_2-alkylacenapthol, ethanethiol, and methanethiol. The

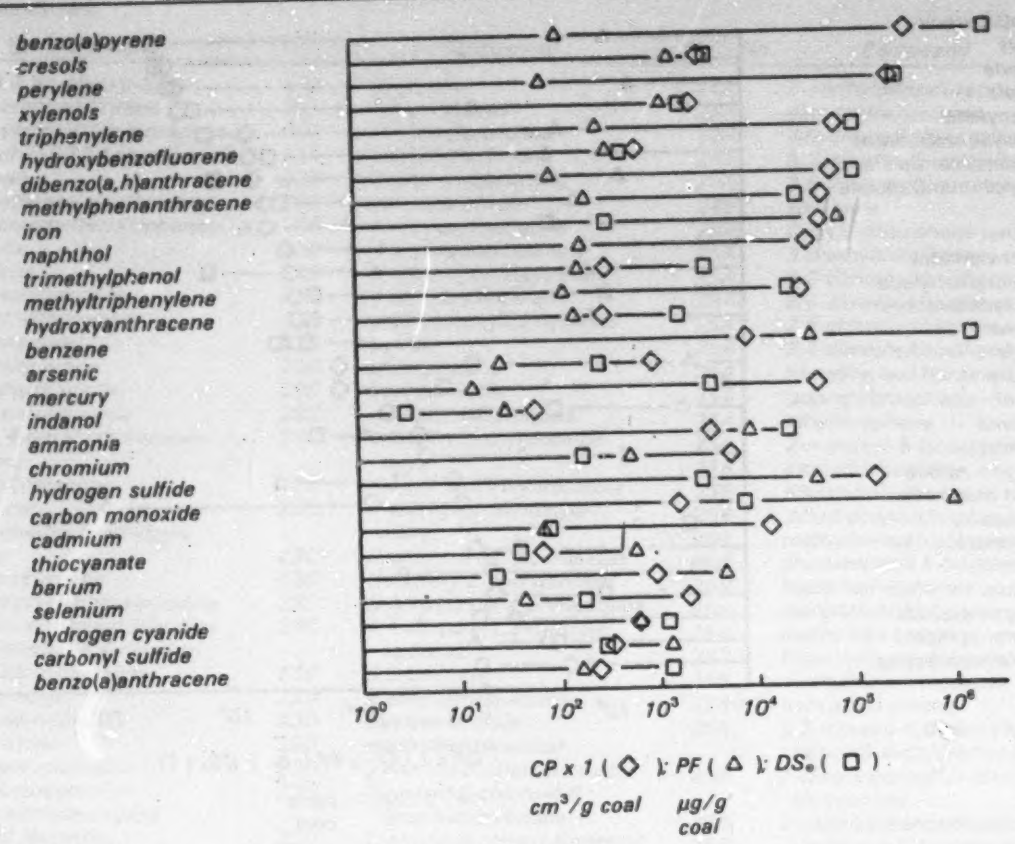

Figure 2. Ecological hazard indices and production levels for potentially hazardous coal gasification pollutants.

phenols added are questionable because of an unjustifiably severe DMEG associated with that class (see following discussion of Figure 5c).

Category discharge severities for MEG categories are shown in Figures 5a-5e, for all streams in all processes. The DS_n values result from summation of discharge severities for maximum concentrations in all streams from Table 1. Trace elements are lumped into a single category, TE. Of the 15 categories listed, categories 18 and 21 have the highest composite discharge severity. A few compounds in a category can account almost entirely for the category's discharge severity. On the other hand, while substances in categories such as 22 do not manifest themselves as individual high priority hazards, the summation of severities of substances in the class gives it a significant total discharge severity.

In Figure 5b, benzene is almost entirely responsible for the DS value of category 15. All but one of the categories in Figure 5a are represented in this figure, primarily because gas streams were emphasized in the sampling and analysis approach for most processes (see Table 1). Also, aerosols and particulates were sampled in gas streams, causing, for example, the high discharge severity of category 21. Gas streams account for all of the apparent hazard in categories 1, 13, 17, and 25 ($DS > 1$).

Figure 5c shows that phenols in aqueous streams overshadow other hazards. However, new water quality criteria[19] have increased recommended control levels for phenol, changing the $DMEG_{h-w}$ from 5 μg/l to 1.5×10^3 μg/l. This should also increase future DMEGs for cresols, xylenols, and other phenolic forms, effectively reducing discharge severity in this category by more than two orders of magnitude.

The same can be said for category 18's contribution to tar hazard in Figure 5d. This leaves polynuclear aromatics of category 21 dominating the tar hazard potential. However, limitations of chemical analysis in determining the data base represented by the source report may cause underestimation of tar hazard. For example, biological assays[19] and chemical analyses of coal gasification tars,[20] published subsequent to formulation of the source report data base, show that amines of category 10, nitrogen heterocyclics of category 23, and sulfur heterocyclics of category 25 have been neglected in terms of their potential hazard. RTI bioassays show that the organic base fraction (including categories 10 and 23) is the most highly mutagenic fraction in some coal tars, even when compared to the polynuclear aromatic fraction.

Potential hazard for solids is entirely contributed by trace elements, as seen in Figure 5e. Trace element hazard potential is almost evenly distributed among stream types, due to the volatility of many trace elements under the high

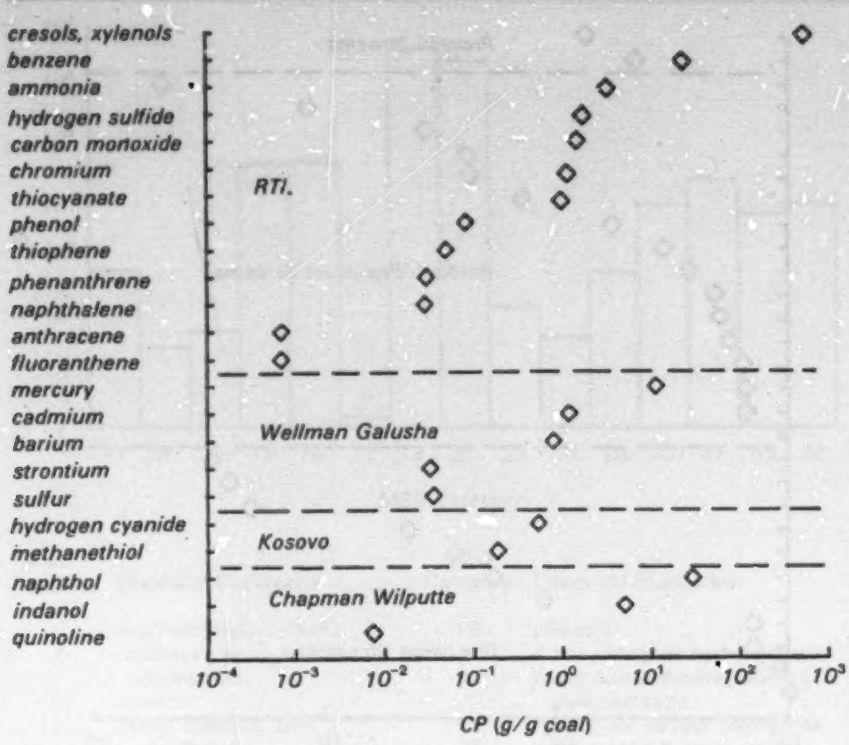

Figure 3. Categorization of pollutant hazards by process type.

temperature conditions of coal gasification.

Figures 6-9 show the main contributors to hazard potential by stream type. Based on discharge severity, more kinds of chemical species are represented in gas streams than for any other streams. The data confirm the widely recognized control problems associated with mercaptans, benzene, polynuclear aromatics (aerosols, particulate), ammonia, hydrogen sulfide, and trace elements. It can be argued that for fuel gas product streams, removal of pollutants to obtain discharge severities below that of carbon monoxide is not justified, since this primary fuel product is not a candidate for removal. However, for noncombustion application, and indeed from a process technology standpoint, a clean product is desirable.

For gases and other streams whose end use is combustion, it may also be argued that the end use provides a satisfactory control technology. In the case of product gas, only sulfur species and trace elements would be excluded by this argument. Some particularly virulent stream concentrations are associated with Figure 6, especially ammonia, benzene, mercaptans, hydrogen sulfide, and C_6 + hydrocarbons. Maximum concentrations for these species were all obtained from samples taken at the Kosovo Lurgi plant.

For liquid stream discharge severities (Figure 7), incorporating anticipated increased DMEGs for phenols would reduce maximum hazard potentials to DS $\simeq 10^{3.5}$. Such substances as polycyclic hydrocarbons in liquid streams obviously indicate inadequate liquid separation of aqueous effluents from tars, oils, and particulates. However, low concentrations of these species significantly reduce their contribution to DS. The data again confirm the importance of such widely recognized contaminants as phenols, ammonia, cyanide/cyanates, and trace elements. It is interesting that chlorine's contribution is not significant for all the data analyzed, and that no legitimate evidence of polychlorinated compounds has been demonstrated. For the worst case of all streams sampled, ammonia hazard was highest in a gas stream, rather than in a liquid stream.

Constituents found in highest concentrations in tar (Figure 8), such as phenanthrene, anthracene, naphthalene, chrysene, and pyrene, contribute minimally to tar hazard potential. Tar hazard is owed to the incredible number of organic constituents represented in trace quantities, only a few of which are shown in the figure. Further definition of compounds outside the classically researched area of fused polycyclic hydrocarbons is needed. The lowest relative concentration of trace elements is found in tar, supporting its candidacy for combustion.

Solids streams are almost entirely represented by coal ash (Figure 9). For this stream, as for gases, some of the commercial gasifiers' maximum concentrations are at levels which strain credulity. For example, levels of antimony, selenium, and mercury greatly exceed maxima reported in any U.S. coal. It is not likely that these highly volatile elements would be concentrated in coal ash. On the other hand, potential hazard from such elements as arsenic is well documented and confirmed by the data. Overall ash hazard appears to be the lowest of any coal gasification stream, although evaluations must ultimately be reviewed in the context of potential control technologies and disposal options.

In conclusion, coal gasification presents potential hazards in all streams of all processes reviewed. The compounds indicated are certainly candidates for first priority control consideration in coal gasification environmental assessment. Single substance, and total, discharge severities approach seven orders of magnitude in a few cases. For a number of substances (where DS $\geq 10^3$), reduction of concentration by more than 99.9 percent is implied—effectively requiring, in many cases, pollutant reduction to nondetectable limits. Such apparent conclusions emphasize the necessity for restating that DMEGs must be applied in a flexible manner, stressing qualitative appraisal. The source report, with its extensive data base, provides a more comprehensive concept of gasification pollutant problems.

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carbon monoxide
hydrogen sulfide
7,12-dimethylbenzo(a)anthracene
xylenols
dibenzo(a,h)anthracene
triphenylene
2,4,6 trimethylphenol
isopropylphenol
C2-alkylphenol
hydroxyanthracene
hydroxybenzofluorene
methylphenanthracene
C2-alkylhydroxypyrene
C5-alkylhydroxyanthracene
1-naphthol
C2-alkylacenaphthol
methyltriphenylene
C2-alkylphenol
cresol
benzo(a)pyrene
perylene
benzene
ethanethiol
ammonia
methanethiol
phenols
mercury
uranium
cyanide

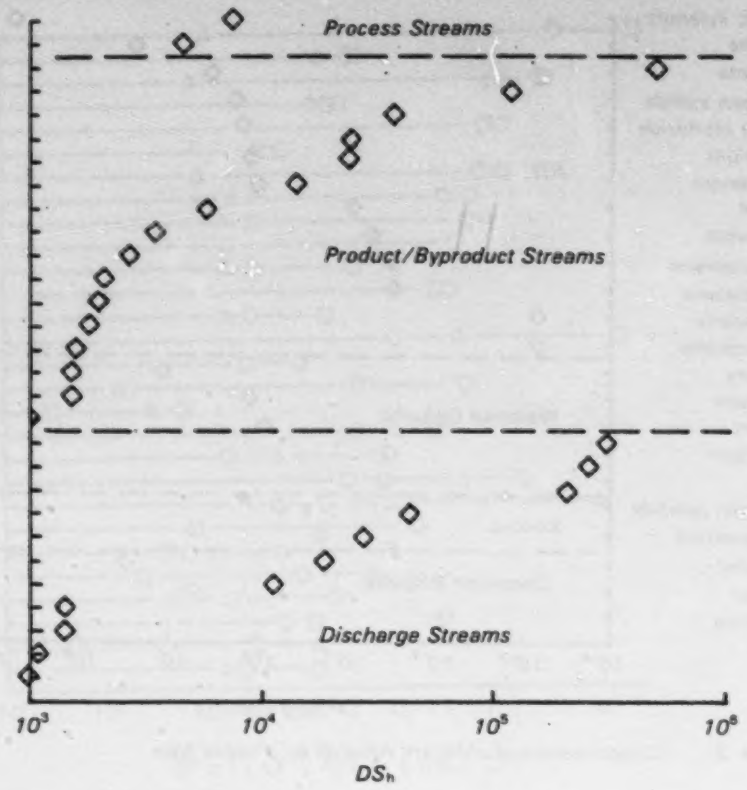

Figure 4. Categorization of pollutant hazards by stream type.

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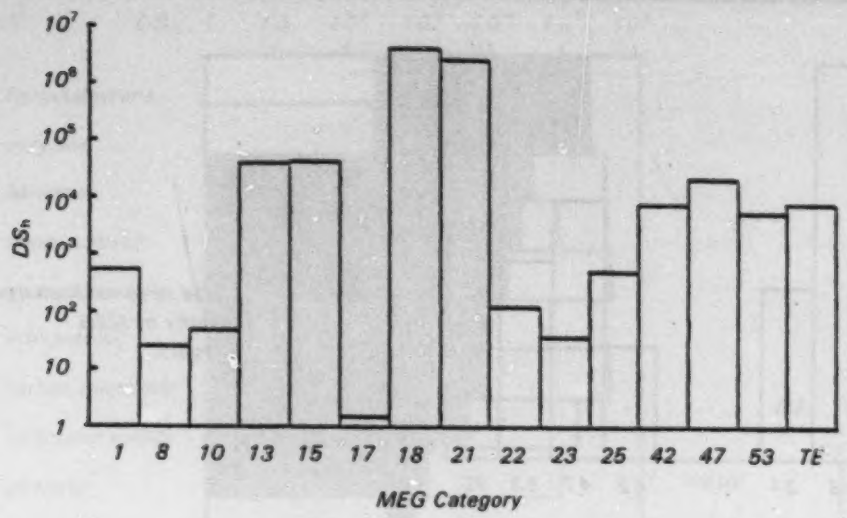

MEG Category	Chemical Substance	MEG Category	Chemical Substance
1	aliphatic hydrocarbons	18	phenols
8	carboxylic acids and derivatives	21	fused polycyclic hydrocarbons
10	amines	22	fused non-alternate polycyclic hydrocarbons
13	thiols, sulfides, and disulfides	23	heterocyclic nitrogen compounds
15	benzene, substituted benzene hydrocarbons	25	heterocyclic S compounds
17	aromatic nitro compounds	42	carbon-free & combined
		47	nitrogen-free & combined
		53	sulfur-free & combined
		TE	trace elements

Figure 5a. *Discharge severity of all streams by MEG category.*

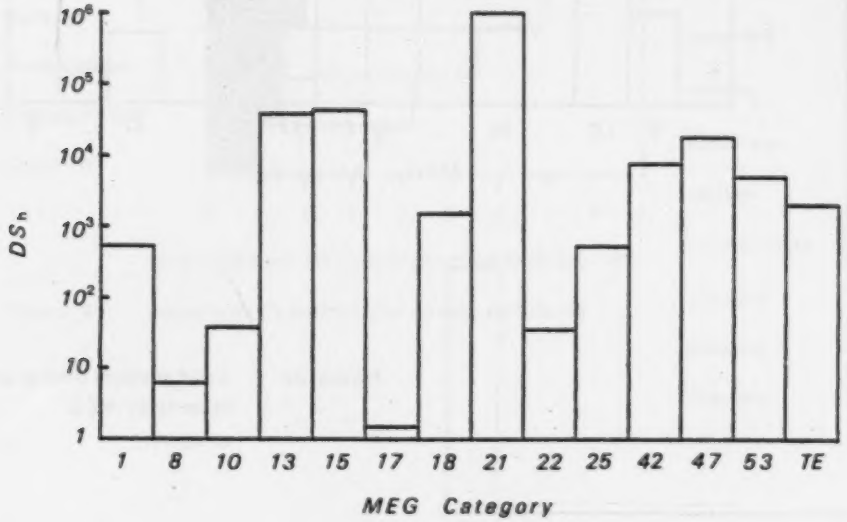

Figure 5b. *Gas streams discharge severity by MEG category.*

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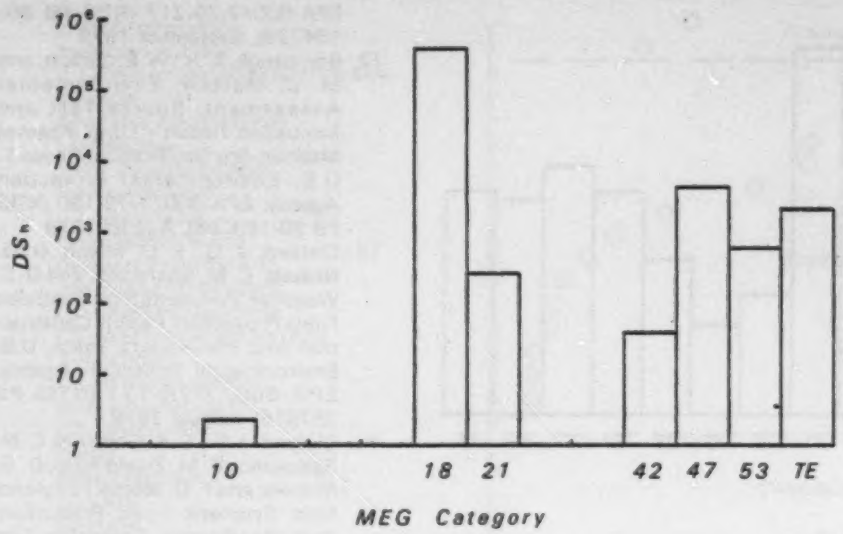

Figure 5c. *Liquid streams discharge severity by MEG category.*

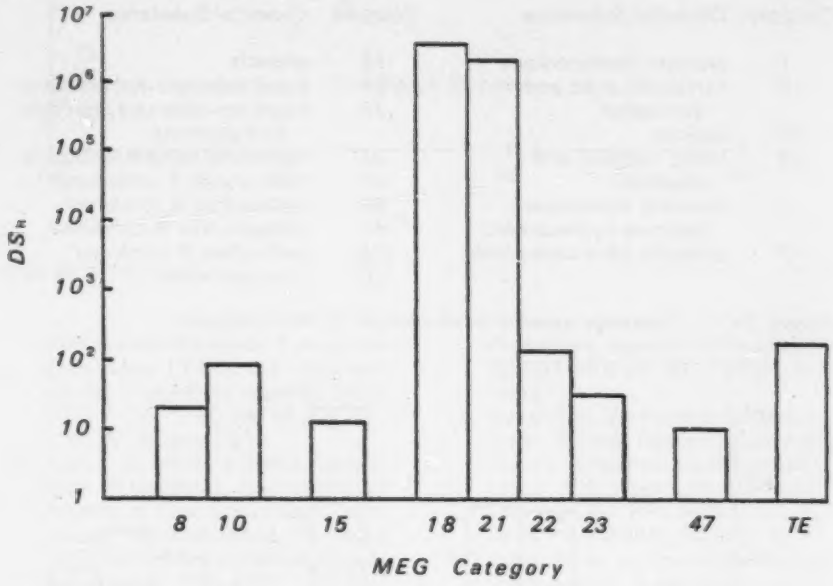

Figure 5d. *Tar stream discharge severity by MEG category.*

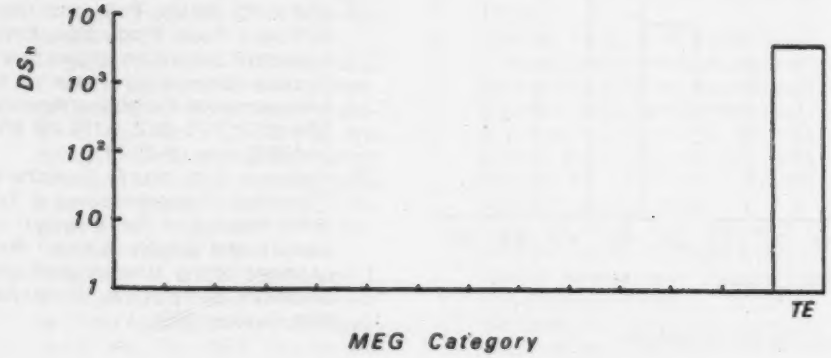

Figure 5e. *Solid streams discharge severity by MEG category.*

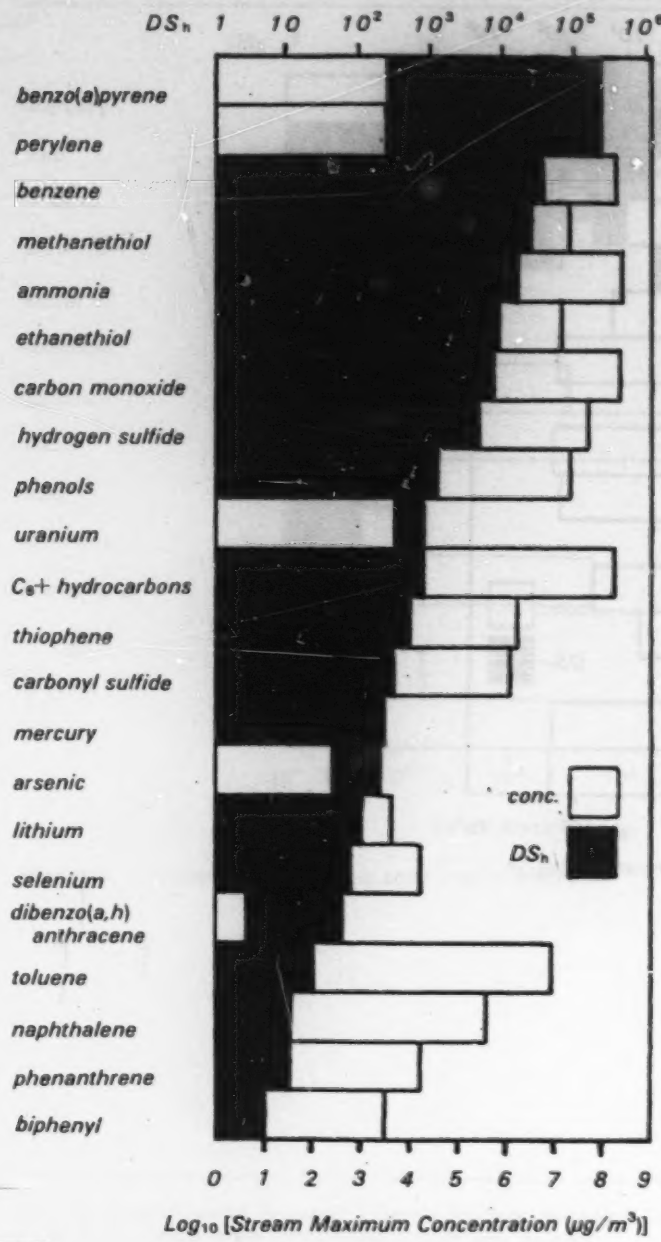

Figure 6. *Potentially hazardous gas stream pollutants.*

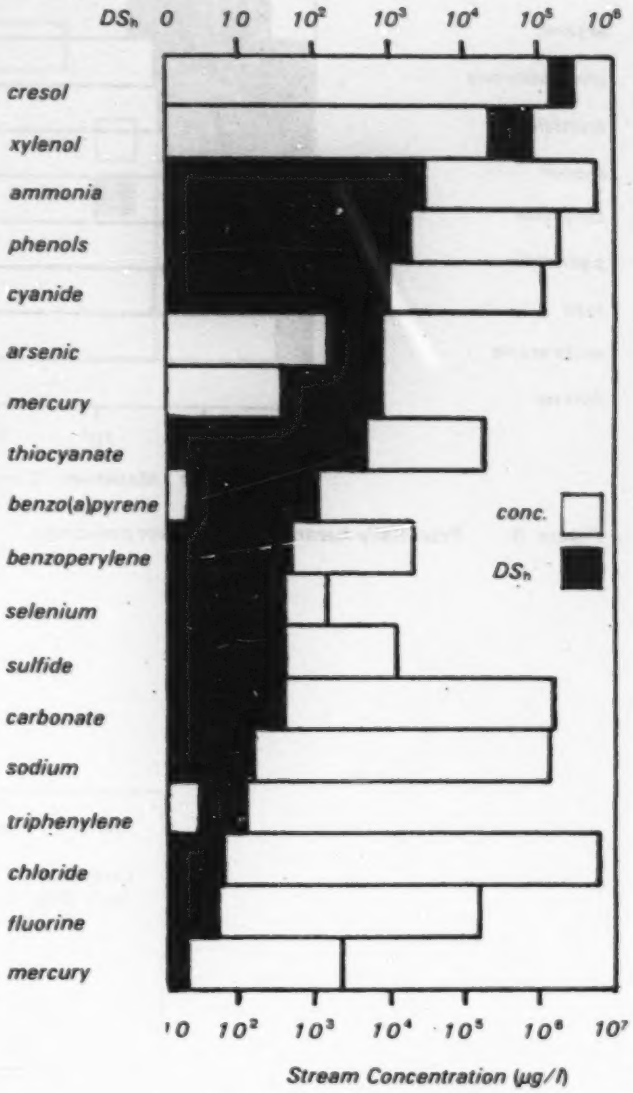

Figure 7. *Potentially hazardous liquid stream pollutants.*

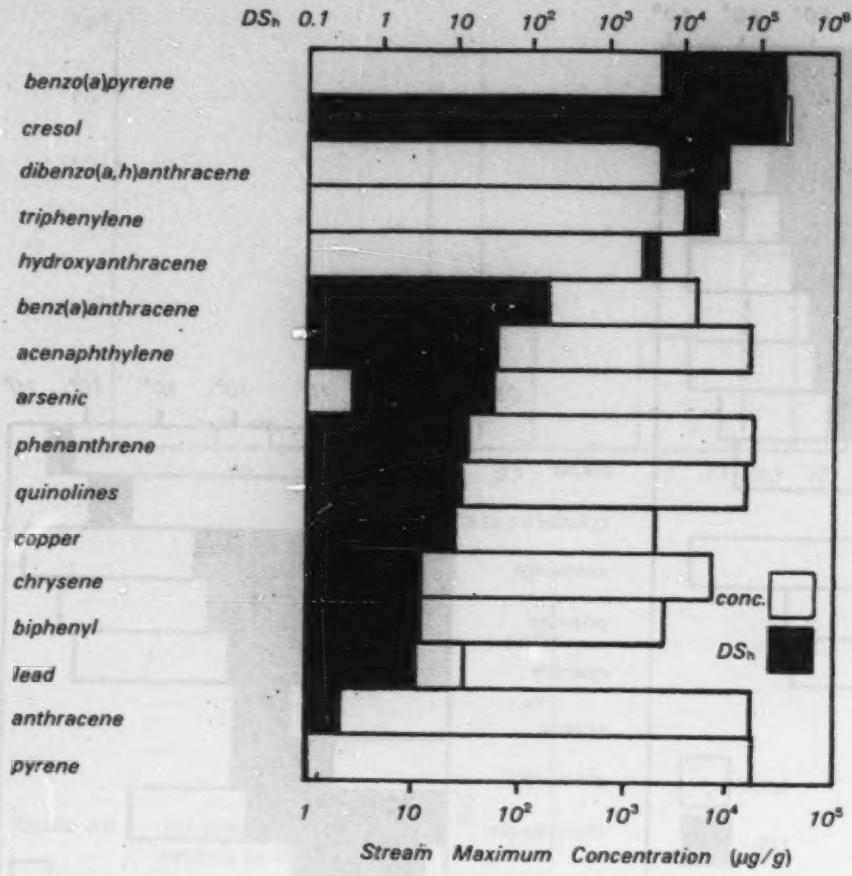

Figure 8. *Potentially hazardous tar stream pollutants.*

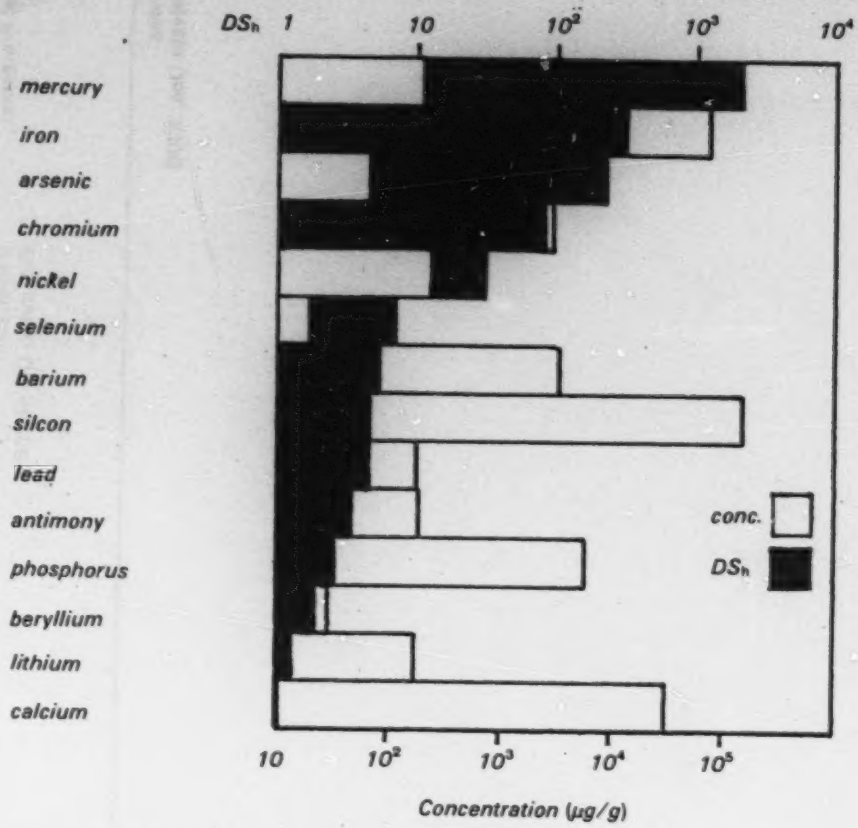

Figure 9. *Potentially hazardous solid stream pollutants.*

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The complete report, entitled "Environmental Hazard Rankings of Pollutants Generated in Coal Gasification Processes," (Order No. PB 81-231 698; Cost: $27.50, subject to change) will be available only from:
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